IN THE CLAIMS:

Amend the claims as follows:

Claims 1-76. (Canceled)

77. (new) A computer-based method for the analysis of the interaction of a molecular structure with a P450 structure, which comprises:

providing a structure comprising a three-dimensional representation of P450 3A4 or a portion of P450 3A4, which representation comprises all or a portion of the coordinates of Table 5 $\pm$ a root mean square deviation from the Cα atoms of not more than 1.5 Å;

providing a molecular structure to be fitted to said P450 3A4 structure or selected coordinates thereof; and

fitting the molecular structure to said P450 3A4 structure.

78. (new) The method of claim 77 wherein said representation further comprises all or a portion of the coordinates of Table 6.

79. (new) The method of claim 77 wherein said selected coordinates include atoms from one or more of the residues of Phe57, Phe108, Phe213, Phe215, Phe219, Phe220, Phe241 and Phe304.

80. (new) The method of claim 77 wherein said selected coordinates include atoms from one or more of the residues of Table 7.

81. (new) The method of claim 80 where said selected coordinates include atoms from one or more of the residues of Table 8.

82. (new) The method of claim 77 which further comprises the steps of:

obtaining or synthesising a compound which has said molecular structure; and

contacting said compound with P450 protein to determine the ability of said compound to interact with the P450.

83. (new) The method of claim 77 which further comprises the steps of:

obtaining or synthesising a compound which has said molecular structure;

forming a complex of a 3A4 P450 protein and said compound; and

analysing said complex by X-ray crystallography to determine the ability of said compound to interact with the P450.

84. (new) The method of claim 77 which further comprises the steps of:

obtaining or synthesising a compound which has said molecular structure; and

determining or predicting how said compound is metabolised by said P450 structure; and

modifying the compound structure so as to alter the interaction between it and the P450.

85. (new) The method of claim 77 wherein the molecular structure to be fitted is in the form of a model of a pharmacophore.

86. (new) The method of claim 77 wherein the three-dimensional representation is a model constructed from all or a portion of the coordinates of Table 1 ± a root mean square deviation from the Cα atoms of less than 0.5Å.

87. (new) The method of claim 86 wherein the model is selected from the group consisting of : (a) a wire-frame model; (b) a chicken-wire model; (c) a ball-and-stick model; (d) a space-filling model; (e) a stick-model; (f) a ribbon model; (g) a snake model; (h) an arrow and cylinder model; and (i) an electron density map; (j) a molecular surface model.

88. (new) A computer-based method for the analysis of molecular structures which comprises:

(a) providing the coordinates of at least two atoms of a P450 3A4 structure as defined in Table 5 ± a root mean square deviation from the Cα atoms of less than 1.5 Å as selected coordinates;

(b) providing the structure of a molecular structure to be fitted to the selected coordinates; and

(c) fitting the structure to the selected coordinates of the P450 3A4 structure.

89. (new) The method of claim 88 wherein the selected coordinates are of at least one of 5, 10, 50, 100, 500 and 1000 atoms.

90. (new) The method of claim 88 wherein the coordinates of Table 5 represent at least a portion of a binding pocket.

91. (new) The method of claim 88 wherein the coordinates of Table 5 comprise at least 2 atoms of the amino acid residues of Table 7.

92. (new) The method of claim 91 wherein the coordinates of Table 5 comprise at least 2 atoms of the amino acid residues of Table 8.

93. (new) A computer-based method of rational drug design comprising:

(a) providing the coordinates of at least two atoms of a P450 3A4 structure as defined in Table 5 $\pm$ a root mean square deviation from the Cα atoms of less than 1.5 Å, as selected coordinates;

(b) providing the structures of a plurality of molecular fragments;

(c) fitting the structure of each of the molecular fragments to the selected coordinates; and

(d) assembling the molecular fragments into a single molecule to form a candidate modulator molecule.

94. (new) The method of claim 93 further comprising the step of:

(a) obtaining or synthesising the molecular fragment or modulator molecule; and

(b) contacting the molecular fragment or modulator molecule with P450 3A4 to determine the ability of the molecular fragment or modulator molecule to interact with P450 3A4.

95. (new) A method for identifying a candidate modulator of P450 3A4 comprising the steps of:

(a) employing a three-dimensional structure of P450 3A4, at least one sub-domain thereof, or a plurality of atoms thereof, to characterise at least one P450 3A4 binding cavity, the three-dimensional structure being defined by atomic coordinate data according to Table 5 $\pm$ a root mean square deviation from the Cα atoms of less than 1.5 Å; and

(b) identifying the candidate modulator by designing or selecting a compound for interaction with the binding cavity.

96. (new) The method of claim 95 further comprising the step of:

(a) obtaining or synthesising the candidate modulator; and

(b) contacting the candidate modulator with P450 3A4 to determine the ability of the candidate modulator to interact with P450 3A4.

97. (new) A computer-based method for identifying a candidate modulator of P450 3A4 comprising the steps of:

employing a three-dimensional structure of P450 3A4, or selected co-ordinates thereof, the three-dimensional structure being defined by atomic coordinate data according to Table 5 $\pm$ a root mean square deviation from the Cα atoms of less than 1.5 Å;

identifying the candidate modulator by designing or selecting a compound for interaction with the binding cavity.